

Spin stiffness and quantum fluctuations in C -type and A -type antiferromagnets

Marcin Raczkowski and Andrzej M. Oleś

Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland
(21 March 2002)

We present a systematic study of quantum fluctuations in the C -type and A -type antiferromagnetic (AF) phases in cubic lattices and in bilayer systems. Using the linear spin-wave theory, we show that the spin stiffness and the quantum corrections to the order parameter and energy obtained for C -AF and A -AF phases decrease with the increasing number of ferromagnetic bonds. Therefore, the quantum spin effects in LaMnO_3 and in LaVO_3 are rather small, suggesting the magnetic moments of ~ 3.91 and $\sim 1.89\mu_B$, respectively. They cannot explain the strong reduction of the magnetic order parameter observed in cubic vanadates. [Published in Phys. Rev. B **66**, 094431 (2002)]

75.30.Ds, 75.30.Et, 75.50.Ee

The undoped transition metal oxides are characterized by large local Coulomb interactions $\propto U$, which lead to several fascinating phenomena such as high-temperature superconductivity and “colossal magnetoresistance”.¹ When the Coulomb interactions dominate over the kinetic energy, the charge fluctuations are quenched and the magnetic properties follow from the effective low-energy superexchange interactions. In some of these systems the orbital degrees of freedom play a role due to the partial filling of (almost) degenerate d orbitals, the superexchange interactions are strongly frustrated,^{2,3} and the quantum effects are enhanced.⁴ These interactions together with the Jahn-Teller effect may induce the orbital ordering below a structural transition and break the cubic symmetry of the perovskite lattice. In such systems, although the crystallographic directions in a three-dimensional (3D) cubic lattice are *a priori* equivalent, one finds magnetic interactions not only of different value, but even of *different sign*, stabilizing C -type or A -type antiferromagnetic (AF) phases.³

One of the best known examples of the non-cubic magnetic interactions in a perovskite system is the A -type AF order observed in LaMnO_3 ,⁵ with ferromagnetic (FM) superexchange within (a, b) planes (J_{ab}) and AF interactions along the c axis (J_c), or in KCuF_3 , an almost perfect one-dimensional (1D) Heisenberg antiferromagnet.⁶ In both above cases the magnetic ordering is supported by the orbital ordering which is induced either by the Jahn-Teller effect,^{7,8} or by the superexchange interactions.^{9,10} Recently it was suggested that the latter contribution dominates,¹⁰ but this issue is still controversial and has to be clarified by future studies. The spin waves in LaMnO_3 have been investigated in great detail and it was established that the AF interactions J_c are weaker than the FM J_{ab} ones,⁹ in good agreement with the experimental data.¹¹

An inverse situation with respect to manganites and cuprates, with AF interactions within (a, b) planes coexisting with FM superexchange along the c -axis, is encountered in the so-called C -AF phase, observed in cubic vanadates: in LaVO_3 below the Néel temperature $T_N \simeq 143$ K,¹² and in YVO_3 at intermediate temper-

atures $77 < T < 116$ K.¹³ Finally, G -type AF order, with cubic symmetry and the magnetic order parameter staggered in all three directions, is found in CaMnO_3 , LaTiO_3 , and also in the low-temperature phase of YVO_3 .¹³ Particularly this last example shows that the type of magnetic order observed in transition metal oxides may be triggered by a delicate balance of magnetic interactions induced by the orbital ordering.

Other examples of non-cubic antiferromagnets are found in bilayer systems, where the effective dimensionality is reduced and the cubic symmetry is explicitly broken by geometry, even when the exchange interactions are AF and identical on the bonds in different crystallographic directions. The G -AF structure is realized in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$,¹⁴ while the bilayer manganites $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ show interesting dependence of the magnetic order on the doping, with FM structure for $x \simeq 0.4$ (Ref. 15) and A -AF structure for $x \simeq 0.48$,¹⁶ separated by a C -AF phase at intermediate doping.¹⁷

The renewed interest in the magnetic properties of transition metal oxides motivates a systematic study of quantum fluctuations in different AF structures. The spin-wave theory was introduced long ago,¹⁸ and high accuracy results of the $1/S$ expansion were presented for a two-dimensional (2D) Heisenberg antiferromagnet.^{19,20} More recently the properties of 2D dimerized models were studied.²¹ However, we are not aware of any systematic investigation of the spin stiffness and the quantum effects in non-cubic systems with different strengths and signs of exchange interactions. In this paper we consider the quantum fluctuations in the AF phases realized in transition metal perovskites, and compare them with those known for the 2D square and 3D cubic lattice. Further motivation comes from the experimental data for numerous systems which could be properly understood only when spin effects would be extracted from the full quantum problem. Therefore, we neglect the orbital fluctuations, and study the spin quantum effects alone in the structures stabilized by the superexchange fixed by a rigid orbital background.

We consider the (effective) 3D Heisenberg model with nearest-neighbor superexchange interactions, J_{ab} in (a, b)

planes and J_c along c axis, between spins S in G -AF, C -AF and A -AF phases, given by

$$\mathcal{H}_{3D} = J_{ab} \sum_{\langle ij \rangle \parallel (a,b)} \mathbf{S}_i \cdot \mathbf{S}_j + J_c \sum_{\langle ij \rangle \parallel c} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

In cubic crystals the G -AF phase is obtained for $J_{ab} > 0$ and $J_c > 0$, while FM interactions stabilize either C -AF phase if $J_c < 0$, or the A -AF phase if $J_{ab} < 0$. Similar phases are possible in the bilayer structures, with the second sum involving only the interlayer bonds. We will investigate the range of parameters with the interlayer coupling $|J_c| \leq 2J_{ab}$, where the ground state is ordered. In contrast, for $J_c/J_{ab} > 2.55$ the magnetic properties are dominated by the singlets which form on interlayer bonds $\langle ij \rangle \parallel c$ axis, the long-range order is lost, and the spin-wave expansion does not apply.²² As a reference system, we also performed calculations for the 2D square lattice with different interactions along the bonds parallel to a and b axis, respectively, described by,

$$\mathcal{H}_{2D} = J_a \sum_{\langle ij \rangle \parallel a} \mathbf{S}_i \cdot \mathbf{S}_j + J_b \sum_{\langle ij \rangle \parallel b} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (2)$$

We assume $J_a > 0$ and study both the G -AF ($J_b > 0$) and C -AF ($J_b < 0$) phase.

We determined the dispersion of spin waves in the spin models given by Eqs. (1) and (2), the quantum corrections to the magnetic order parameter $\langle S^z \rangle$, and to the ground state energy $E = \langle \mathcal{H}_{3D} \rangle$ ($E = \langle \mathcal{H}_{2D} \rangle$) using the linear spin-wave theory (LSWT) in the leading $1/S$ order. First we transform the spin operators at the sites $j \in B$ sublattice: $S_j^\pm \rightarrow S_j^\mp$, $S_j^z \rightarrow -S_j^z$, which removes spins down $\langle S_j^z \rangle_0 = -S$ of the Néel state. Next we introduce bosonic operators $\{a_i^\dagger, a_i\}$, and use the lowest order of the Holstein-Primakoff transformation:²³

$$S_i^z = S - a_i^\dagger a_i, \quad S_i^+ \simeq \sqrt{2S} a_i, \quad S_i^- \simeq \sqrt{2S} a_i^\dagger. \quad (3)$$

The excitations are derived from the equations of motion for the energy-dependent Green's functions,^{24,25}

$$E \langle \langle a_i | a_j^\dagger \rangle \rangle = \frac{1}{2\pi} \delta_{ij} + \langle \langle [a_i, \mathcal{H}_{3D}] | a_j^\dagger \rangle \rangle. \quad (4)$$

After the Fourier transformation the spin waves are found by a Bogoliubov transformation which diagonalizes a 2×2 dynamical matrix at each \mathbf{k} point. The positive magnon energies for the 3D G -AF, C -AF and A -AF phase are:

$$\omega_G(\mathbf{k}) = 2S \{ (2J_{ab} + J_c)^2 - [2J_{ab}\gamma_+(\mathbf{k}) + J_c\gamma_z(\mathbf{k})]^2 \}^{1/2}, \quad (5)$$

$$\omega_C(\mathbf{k}) = 2S \{ [2J_{ab} + |J_c|(1 - \gamma_z(\mathbf{k}))]^2 - 4J_{ab}^2\gamma_+^2(\mathbf{k}) \}^{1/2}, \quad (6)$$

$$\omega_A(\mathbf{k}) = 2S \{ [2|J_{ab}|(1 - \gamma_+(\mathbf{k})) + J_c]^2 - J_c^2\gamma_z^2(\mathbf{k}) \}^{1/2}, \quad (7)$$

where $\gamma_+(\mathbf{k}) = \frac{1}{2}(\cos k_x + \cos k_y)$ and $\gamma_z(\mathbf{k}) = \cos k_z$ are \mathbf{k} -dependent structure factors. The corresponding magnon energies for the bilayer systems are:

$$\omega_G^\parallel(\mathbf{k}) = S \{ (4J_{ab} + J_c)^2 - [4J_{ab}\gamma_+(\mathbf{k}) + \lambda J_c]^2 \}^{1/2}, \quad (8)$$

$$\omega_C^\parallel(\mathbf{k}) = S \{ [4J_{ab} + |J_c|(1 - \lambda)]^2 - 16J_{ab}^2\gamma_+^2(\mathbf{k}) \}^{1/2}, \quad (9)$$

$$\omega_A^\parallel(\mathbf{k}) = S \{ [4|J_{ab}|(1 - \gamma_+(\mathbf{k})) + J_c]^2 - \lambda^2 J_c^2 \}^{1/2}, \quad (10)$$

where $\lambda = \pm 1$ corresponds to $k_z = 0, \pi$, i.e., to the symmetric and antisymmetric interlayer modes, respectively. The magnon energies for the G -AF and C -AF phase in the 2D case are:

$$\omega_G^{2D}(\mathbf{k}) = 2S \{ (J_a + J_b)^2 + [J_a\gamma_x(\mathbf{k}) + J_b\gamma_y(\mathbf{k})]^2 \}^{1/2}, \quad (11)$$

$$\omega_C^{2D}(\mathbf{k}) = 2S \{ [J_a + |J_b|(1 - \gamma_y(\mathbf{k}))]^2 - J_a^2\gamma_x^2(\mathbf{k}) \}^{1/2}, \quad (12)$$

with $\gamma_x(\mathbf{k}) = \cos k_x$, and $\gamma_y(\mathbf{k}) = \cos k_y$.

The size of quantum fluctuation corrections to the classical order parameter $\langle S_i^z \rangle_0 = S$, and the intersite spin fluctuations $\propto \langle S_i^- S_j^+ \rangle$ which modify the energy, determine the stability of the classical phases. One finds that the order parameter for $i \in A$ sublattice is reduced by local quantum fluctuations,

$$\langle S_i^z \rangle = S - \langle S_i^- S_i^+ \rangle = S - \delta \langle S^z \rangle, \quad (13)$$

and the local correlation function $\langle S_i^- S_i^+ \rangle$ is determined by the Green's function $\langle \langle a_{\mathbf{k}} | a_{\mathbf{k}}^\dagger \rangle \rangle$ by,²⁵

$$\langle S_i^- S_i^+ \rangle = \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} d\omega \mathcal{I}(\mathbf{k}, \omega) \frac{1}{\exp(\beta\omega) - 1}, \quad (14)$$

where $\beta = 1/k_B T$, N is the number of sites, and

$$\begin{aligned} \mathcal{I}(\mathbf{k}, \omega) &= 2 \text{Im} \langle \langle a_{\mathbf{k}} | a_{\mathbf{k}}^\dagger \rangle \rangle_{\omega - i\epsilon} \\ &= \sum_{\nu} \mathcal{A}^{(\nu)}(\mathbf{k}) \delta(\omega - \omega_{\mathbf{k}}^{(\nu)}) \end{aligned} \quad (15)$$

is the spectral density of spin excitations, with the operator $a_{\mathbf{k}}$ being a Fourier transform of a_i . The quantum corrections are found by taking $T \rightarrow 0$ limit of Eq. (14), where the averages $\langle S_i^- S_i^+ \rangle$ are determined from the spectral weights $\mathcal{A}^{(\nu)}(\mathbf{k})$ in Eq. (15) of the excitations at negative frequencies, and therefore,

$$\delta \langle S^z \rangle = \frac{1}{N} \sum_{\mathbf{k}} \sum_{\nu < 0} \mathcal{A}^{(\nu)}(\mathbf{k}). \quad (16)$$

Thus, using Eqs. (15) and (16) one obtains the quantum corrections $\delta \langle S^z \rangle$ for the 3D phases:

$$\delta \langle S^z \rangle_G = S \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{2J_{ab} + J_c}{\omega_G(\mathbf{k})} - \frac{1}{2}, \quad (17)$$

$$\delta \langle S^z \rangle_C = S \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{2J_{ab} + |J_c|[1 - \gamma_z(\mathbf{k})]}{\omega_C(\mathbf{k})} - \frac{1}{2}, \quad (18)$$

$$\delta \langle S^z \rangle_A = S \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{2|J_{ab}||1 - \gamma_+(\mathbf{k})| + J_c}{\omega_A(\mathbf{k})} - \frac{1}{2}, \quad (19)$$

with magnon dispersions given by Eqs. (5)–(7). The quantum corrections for the bilayer structures and for the square lattice can be obtained in a similar way – they involve 2D integrations over the respective excitation spectra, and, in addition, the summation over the symmetric and antisymmetric modes for the bilayer system.

The quantum corrections δE to the ground state energy per site, $E = E_0 - \delta E$, where E_0 is the energy found using the classical state, were obtained by integrating the excitation spectra $\omega_M(\mathbf{k})$, with $M = A, C, G$. For instance, for 3D systems one finds $E_0 = -(2|J_{ab}| + |J_c|)S^2$, and

$$\delta E = (2|J_{ab}| + |J_c|)S - \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \omega_M(\mathbf{k}). \quad (20)$$

In order to compare the systems of different dimensionality we use below the relative energy correction $S(\delta E/E_0)$ as a measure of the quantum correction to the ground state energy. For the 3D AF systems with $|J_{ab}| = |J_c| = J$ (or for the 2D systems with $|J_a| = |J_b| = J$) the relative energy correction $\delta E/E_0$ can be expressed by,

$$\frac{\delta E}{E_0} = \frac{\gamma}{zS}, \quad (21)$$

where z is the number of nearest neighbors, and the coefficient $\gamma > 0$ provides a measure of quantum effects. It depends on the system dimensionality, on lattice type, and on the type of AF order. Therefore, we write the ground state energy as follows:²³

$$E = -\frac{1}{2}zJS^2 \left(1 + \frac{\gamma}{zS}\right). \quad (22)$$

Consider first a cubic crystal with equal strength of AF and FM superexchange interactions ($|J_{ab}| = |J_c| = J$).

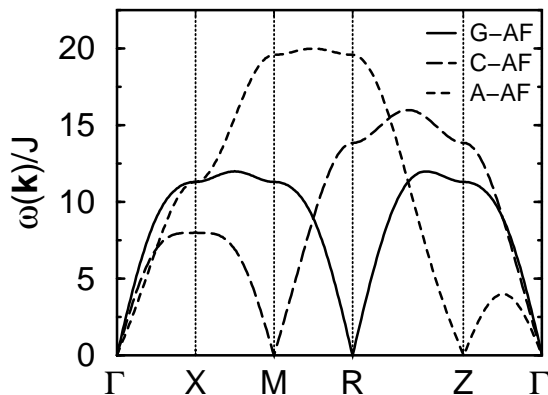


FIG. 1. The spin-wave dispersions as obtained within the LSWT in the G -AF, C -AF and A -AF phases along the main directions of the 3D BZ for a simple cubic lattice, with equal AF and FM exchange interactions ($|J_{ab}| = |J_c| = J$). We have used the standard labels for high-symmetry points: $\Gamma = (0, 0, 0)$, $X = (\pi, 0, 0)$, $M = (\pi, \pi, 0)$, $R = (\pi, \pi, \pi)$, and $Z = (0, 0, \pi)$.

The spin-wave excitations with positive energies are presented in Fig. 1 along the high-symmetry directions of the 3D Brillouin zone (BZ). One finds an expected Goldstone mode with $\omega_M(\mathbf{k}) = 0$ at $R = (\pi, \pi, \pi)$, $M = (\pi, \pi, 0)$, and $Z = (0, 0, \pi)$ point for G -AF, C -AF and A -AF phase, respectively. It corresponds to the vector in the reciprocal space which couples two spin excitations in a given AF structure. The spin excitations are linear near the Goldstone mode, $\omega_M(\mathbf{k}) \simeq Dk$, and close to the Γ point in each AF structure, and the spin-wave stiffness constant D is *isotropic*, being the same for any cubic direction, in spite of the different signs of superexchange constants. Note also that the width of the magnon dispersion increases with the increasing number of FM bonds, and would be the largest and equal to $24J$ for the cubic FM phase, with equal FM exchange interactions in all three directions (not shown). Increasing overall dispersion $\omega_M(\mathbf{k})$ in Eq. (20) reduces the quantum correction δE when the number of FM bonds increases.

We compare the quantum effects given by Eqs. (16) and (21) for different systems listed in Table I. The values obtained for 2D and 3D G -AF phases reproduce the known results given by Mattis.²³ Both $\delta\langle S^z \rangle$ and δE are reduced when some of the bonds are FM. When the dimensionality is fixed, the quantum corrections decrease in a systematic way with the increasing number of FM interactions, from the G -AF to A -AF order.²⁶ A somewhat counterintuitive result is that at the same time the stiffness constant D is enhanced only by the AF interactions, while it *decreases* with the increasing number of FM bonds for all systems: the 3D cubic (see Fig. 1), 2D square, as well as for the bilayer structure (Table I). Thus, the magnon energy increases slower with k near the Γ point by a factor $1/\sqrt{3}$ in A -AF than in G -AF phases. Further, for a given magnetic structure the quantum corrections $\delta\langle S^z \rangle$ and $S(\delta E/E_0)$ gradually *decrease* when the dimensionality of the system *increases* from a 2D square lattice throughout a bilayer system to a 3D cubic lattice (Table I). In the bilayer case an isotropic

TABLE I. The quantum corrections to the magnetic order parameter $\delta\langle S^z \rangle$ and to the ground state energy δE , and the stiffness constant D , as obtained in the LSWT for the phases with isotropic low-energy spin excitations $\omega_M(\mathbf{k}) \simeq Dk$, with $M = G, C, A$. Parameters: $|J_{ab}| = |J_c| = J$ for the 2D and 3D AF phases, and $|J_{ab}| = |J_c|/2 = J$ in the bilayer systems.

lattice	AF phase	$\delta\langle S^z \rangle$	$S(\delta E/E_0)$	$D/2JS$
2D square	G -AF	0.1966	0.1580	$\sqrt{2}$
	C -AF	0.1214	0.0835	1
bilayer	G -AF	0.1589	0.1373	$\sqrt{3}$
	C -AF	0.1069	0.0743	$\sqrt{2}$
	A -AF	0.0859	0.0825	1
3D cubic	G -AF	0.0783	0.0971	$\sqrt{3}$
	C -AF	0.0565	0.0662	$\sqrt{2}$
	A -AF	0.0318	0.0340	1

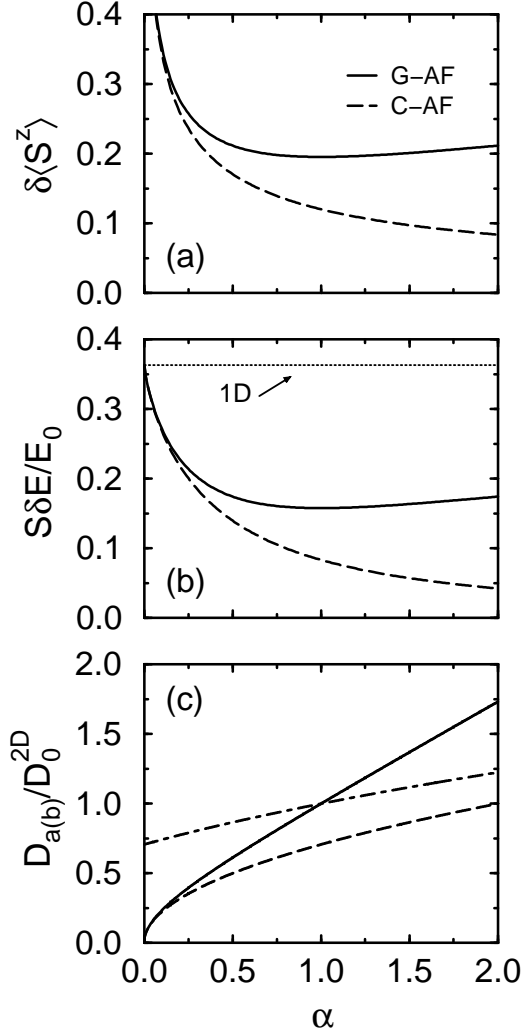


FIG. 2. Quantum corrections to: (a) the magnetic order parameter $\delta\langle S^z \rangle$, and (b) energy $S(\delta E/E_0)$, obtained in the LSWT as functions of $\alpha = |J_b|/J_a$ for the *G*-AF and *C*-AF 2D phase. Part (c) shows the stiffness constants: D_b and D_a for *G*-AF phase (solid and dot-dashed line), and D_b for *C*-AF (long-dashed line), normalized to the value $D_0^{2D} = 2\sqrt{2}JS$ obtained for the *G*-AF phase with $J_a = J_b$. The LSWT result for $S(\delta E/E_0)$ in the 1D model is shown in (b) by dotted line.

stiffness constant is obtained only when the interlayer superexchange interaction is larger by a factor of two than the respective intralayer interactions, i.e., $|J_{ab}| = |J_c|/2 = J$, which simulates the missing second neighbor of each atom along the *c* axis.

The long-range order, with $\langle S^z \rangle > 0$ ($\delta\langle S^z \rangle < 0.5$ for $S = 1/2$) [see Fig. 2(a)], is stabilized within the LSWT in quasi-1D systems realized on a 2D square lattice already by relatively small interchain couplings, $|J_b|/J_a \simeq 0.15$. Qualitatively the values of $\delta\langle S^z \rangle$ and $\delta E/E_0$ [Fig. 2(b)] behave in a similar way; they both decrease for the *C*-AF phase, while the quantum corrections reach a minimum for an isotropic 2D antiferromagnet at $J_b = J_a$ in the

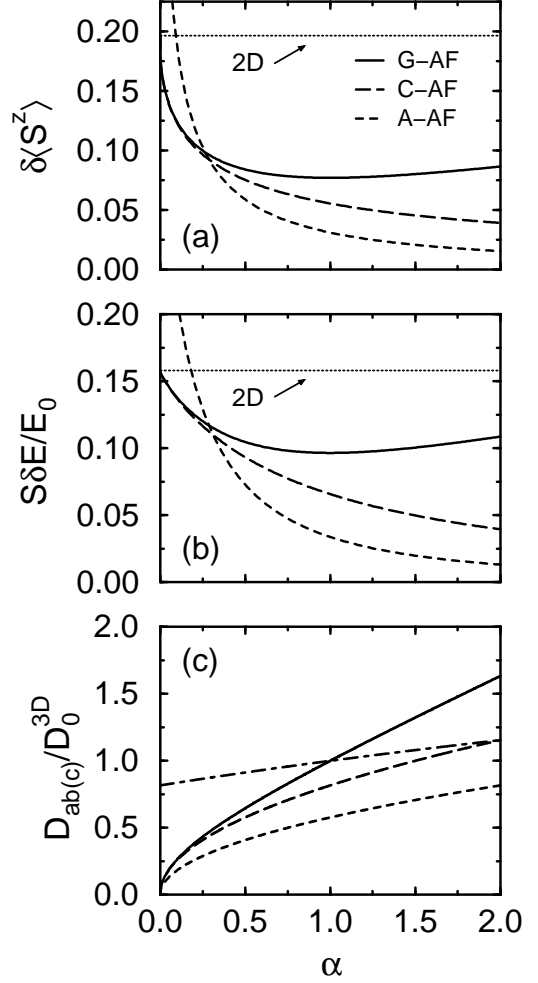


FIG. 3. Quantum corrections as in Fig. 2, but for the 3D AF phases, and with $\alpha = |J_c|/J_{ab}$ ($\alpha = |J_{ab}|/J_c$) for the *G*- and *C*-AF phase (*A*-AF phase). Dotted lines show the values of $\delta\langle S^z \rangle$ (a) and $S\delta E/E_0$ (b), obtained within the LSWT for the isotropic 2D square lattice. Part (c) shows the stiffness constants D_γ normalized to $D_0^{3D} = 2\sqrt{3}JS$ obtained for the *G*-AF phase with cubic symmetry of exchange interactions: D_c and D_{ab} (solid and dot-dashed line) for *G*-AF phase; D_c for *C*-AF phase (long-dashed line), and D_{ab} for *A*-AF phase (dashed line).

G-AF phase, and next increase again for $\alpha > 1$ when a stronger AF interaction occurs along the *b* axis.

The magnon stiffness increases when the (either AF or FM) interactions along the *b* axis $|J_b|$ increase, and one finds $D_b/D_0^{2D} \simeq \sqrt{\alpha}/2$ for small $\alpha = |J_b|/J_a$ [Fig. 2(c)], with $D_0^{2D} = 2\sqrt{2}JS$ obtained in a *G*-AF phase with cubic symmetry. However, the behavior of the *G*-AF and *C*-AF phase is qualitatively different. First of all, the value of D_a increases with J_b in the *G*-AF phase, while it remains constant ($D_a/D_0^{2D} = 1/\sqrt{2}$) in the *C*-AF phase. Second, except for the asymptotic regime of $\alpha < 0.3$, the values of D_b are considerably lower in the *C*-AF phase

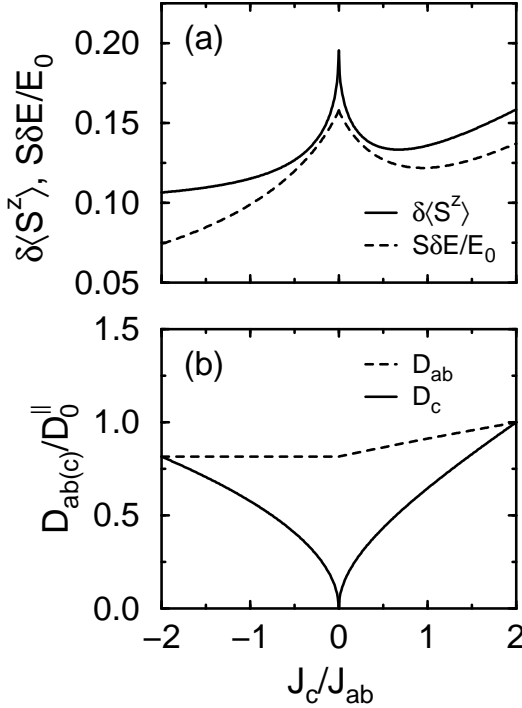


FIG. 4. Quantum corrections (a) to the magnetic order parameter $\delta\langle S^z \rangle$ (solid line), and to the ground state energy $S\delta E/E_0$ (dashed line), and (b) the stiffness constants D_c and D_{ab} (solid and dashed line) for an AF bilayer system with $J_{ab} > 0$, as functions of the interlayer coupling J_c/J_{ab} , in units of $D_0^\parallel = 2\sqrt{3}JS$ (see Table I).

than those in the G -AF phase.

Next we consider C -AF and A -AF order in 3D systems with increasing FM interactions and compare them with the G -AF phase (Fig. 3). Both $\delta\langle S^z \rangle$ and $\delta E/E_0$ decrease rapidly in G -AF phase with increasing $\alpha = J_c/J_{ab}$ in the regime of $0 < \alpha < 0.5$, while for $\alpha > 0.5$ the quantum effects are reduced stronger by the FM bonds which make the magnetic order in the C -AF phase more classical than in the G -AF phase. The values of $\delta\langle S^z \rangle$ and $\delta E/E_0$ increase again for $\alpha > 1$ in the G -AF phase as the system starts to approach a quasi-1D regime with enhanced quantum fluctuations. In the A -AF phase the strongest quantum fluctuations are obtained for small $\alpha = |J_{ab}|/J_c$, where the AF chains along c axis are weakly coupled. However, for $\alpha > 0.3$ the quantum corrections are already smaller than those in the C -AF phase, and further decrease with increasing $\alpha = J_c/J_{ab}$, i.e., when the FM interactions along the c axis get stronger.

The stiffness constants D_{ab} and D_c shown in Fig. 3(c) increase with increasing α in all cases, proving that the increasing exchange interactions cause magnons to harden. For weak interactions along the c axis one finds $D_c/D_0^{3D} \simeq \sqrt{2\alpha/3}$ for G - and C -AF phase, and $D_{ab}/D_0^{3D} \simeq \sqrt{\alpha/3}$ for A -AF phase, where $D_0^{3D} = 2\sqrt{3}JS$ is obtained in a G -AF phase with cubic symmetry. We note that both D_c and D_{ab} increase when J_c

is increased in the G -AF phase. In contrast, the stiffness constants: D_{ab} in the C -AF phase, and D_c in the A -AF phase, are not influenced by the increasing FM interactions (J_c and J_{ab} , respectively), and one finds: $D_{ab}/D_0^{3D} = \sqrt{2/3}$ and $D_c/D_0^{3D} = 1/\sqrt{3}$ in the C -AF and A -AF phase. This illustrates a general rule – when the AF interactions increase, the spin stiffness increases both along the AF and FM bonds. In contrast, the spins on the FM bonds cannot fluctuate and thus the changes of FM interactions do not modify the spin stiffness along the AF bonds.

The dependence of the quantum corrections and the stiffness constants on the interlayer coupling $\propto J_c$ in the bilayer system is summarized in Fig. 4. As in the 3D case (Fig. 3), the increasing interlayer coupling gives a fast crossover from a system of two independent planes to a bilayer system with reduced values of $\delta\langle S^z \rangle$ and $\delta E/E_0$ [Fig. 4(a)]. It is quite remarkable that the effect of finite and small J_c is almost identical for the AF and FM interaction in the regime of $|J_c/J_{ab}| < 0.3$, and the quantum corrections decrease simply due to the dimensional crossover. Only at $|J_c/J_{ab}| > 0.3$ the G -AF and C -AF phase start to differ: the quantum corrections pass through a minimum and increase again due to the AF interlayer coupling ($J_c > 0$) which favors singlet states on these bonds in the G -AF phase, while they steadily decrease when the FM interlayer coupling ($J_c < 0$) gets stronger in the C -AF phase. Similar as in the 3D case, $D_c/D_0^\parallel \simeq \sqrt{\alpha/3}$ in the regime of small $\alpha = |J_c|/J_{ab} < 0.3$, where $D_0^\parallel = 2\sqrt{3}JS$, found for the G -AF phase at $J_c = 2J_{ab}$, is used as a unit. In the C -AF phase the value of $D_{ab} = \sqrt{2/3}D_0^\parallel$ is independent of J_c , while it approaches $D_{ab} = D_0^\parallel$ in the G -AF phase when $|J_c| \rightarrow 2J_{ab}$. Finally, as expected, the quantum corrections in the A -AF bilayer phase increase with increasing AF interlayer coupling $J_c > 0$, and become even larger than those in the C -AF phase for sufficiently large J_c . One finds equal reduction of the order parameter $\delta\langle S^z \rangle \simeq 0.095$ in both phases at $|J_c/J_{ab}| \simeq 2.46$.

The present study shows that the spin quantum corrections due to spin fluctuations are small both in the A -AF phase of LaMnO_3 , and in the C -AF phases of LaVO_3 and YVO_3 . Indeed, large magnetic moments $\sim 3.87\mu_B$ measured in LaMnO_3 (see Ref. 11) are almost perfectly reproduced by the present calculation which gives the moment $\langle M \rangle \simeq 2\mu_B \langle S^z \rangle \simeq 3.91\mu_B$ for spin $S = 2$ and for the experimental ratio of $|J_{ab}|/J_c = 1.43$. In contrast, the strong reduction of the order parameter in LaVO_3 (to $\sim 1.3\mu_B$ ¹²) and YVO_3 (to $\sim 1.0\mu_B$ at finite temperature $T \simeq 85$ K¹³) cannot be explained by rather weak quantum spin effects, reducing the order parameter only down to $\sim 1.89\mu_B$ for spin $S = 1$ and $|J_c|/J_{ab} \simeq 1$ at $T = 0$. This result indicates that the quantum effects due to *orbital fluctuations* are stronger and dominate the behavior of the t_{2g} systems with degenerate orbitals.²⁷

Summarizing, we have shown that the quantum cor-

rections to the order parameter and to the ground state energy *decrease* systematically with the *increasing* number and strength of FM bonds, from *G*-AF through *C*-AF to *A*-AF phase, both in the 3D cubic lattice and in the bilayer system. This shows that the AF interactions *dominate* in the non-cubic antiferromagnets. Indeed, when the interactions are AF along only *one or two* cubic directions, their increase causes the increase of the spin stiffness and of the quantum fluctuations along *all three* cubic directions.

ACKNOWLEDGMENTS

This work was financially supported by the Polish State Committee of Scientific Research (KBN), Project No. 5 P03B 055 20.

-
- ¹ For a review see: M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
- ² Y. Tokura and N. Nagaosa, Science **288**, 462 (2000); A. M. Oleś, M. Cuoco, and N. B. Perkins, in *Lectures on the Physics of Highly Correlated Electron Systems IV*, edited by F. Mancini, AIP Conf. Proc. No. 527 (AIP, New York, 2000), pp. 226-380.
- ³ A. M. Oleś, Acta Phys. Polon. B **32**, 3303 (2001).
- ⁴ L. F. Feiner, A. M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).
- ⁵ E. O. Wollan and W. C. Koehler, Phys. Rev. **100**, 545 (1955).
- ⁶ S. E. Nagler, D. A. Tennant, R. A. Cowley, T. G. Perring, and S. K. Satija, Phys. Rev. B **44**, 12361 (1991); D. A. Tennant, T. G. Perring, R. A. Cowley, and S. E. Nagler, Phys. Rev. Lett. **70**, 4003 (1993); D. A. Tennant, R. A. Cowley, S. E. Nagler, and A. M. Tsvelik, Phys. Rev. B **52**, 13368 (1995); B. Lake, D. A. Tennant, S. E. Nagler, Phys. Rev. Lett. **85**, 832 (2000).
- ⁷ T. Hotta, S. Yunoki, M. Mayr, and E. Dagotto, Phys. Rev. B **60**, R15009 (1999).
- ⁸ Y.-S. Su, T. A. Kaplan, S. D. Mahanti, and J. F. Harrison, Phys. Rev. B **61**, 1324 (2000).
- ⁹ L. F. Feiner and A. M. Oleś, Phys. Rev. B **59**, 3295 (1999).
- ¹⁰ S. Okamoto, S. Ishihara, and S. Maekawa, Phys. Rev. B **65**, 144403 (2002).
- ¹¹ F. Moussa, M. Hennen, J. Rodriguez-Carvajal, M. Houdeden, L. Pinsard, and A. Revcolevschi, Phys. Rev. B **54**, 15149 (1996); K. Hirota, N. Kaneko, A. Nishizawa, and Y. Endoh, J. Phys. Soc. Jpn. **65**, 3736 (1996).
- ¹² H. C. Nguyen and J. B. Goodenough, Phys. Rev. B **52**, 324 (1995); S. Miyasaka, T. Okuda, and Y. Tokura, Phys. Rev. Lett. **85**, 5388 (2000).
- ¹³ Y. Ren, T. T. M. Palstra, D. I. Khomskii, A. A. Nugroho, A. A. Menovsky, and G. A. Sawatzky, Phys. Rev. B **62**, 6577 (2000); M. Noguchi, A. Nakazawa, S. Oka, T. Arima, Y. Wakabayashi, H. Nakao, and Y. Murakami, *ibid.* **62**, R9271 (2000).
- ¹⁴ M. A. Kastner, R. J. Birgeneau, G. Shirane, and Y. Endoh, Rev. Mod. Phys. **70**, 897 (1998).
- ¹⁵ T. G. Perring, D. T. Adroja, G. Chaboussant, G. Aeppli, T. Kimura, and Y. Tokura, Phys. Rev. Lett. **87**, 217201 (2001); K. Hirota, S. Ishihara, H. Fujioka, M. Kubota, H. Yoshizawa, Y. Moritomo, Y. Endoh, and S. Maekawa, Phys. Rev. B **65**, 064414 (2002).
- ¹⁶ A. Koizumi, S. Miyaki, Y. Kakutani, H. Koizumi, N. Hirao, K. Makoshi, N. Sakai, K. Hirota, and Y. Murakami, Phys. Rev. Lett. **86**, 5589 (2001).
- ¹⁷ Y. D. Chuang, A. D. Gromko, D. S. Dessau, T. Kimura, and Y. Tokura, Science **292**, 1509 (2001).
- ¹⁸ P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, *ibid.* **87**, 568 (1952); T. Oguchi, *ibid.* **117**, 117 (1960).
- ¹⁹ M. Takahashi, Phys. Rev. B **40**, 2494 (1989).
- ²⁰ G. E. Castilla and S. Chakravarty, Phys. Rev. B **43**, 13687 (1991); Z. Weihong and C. J. Hamer, Phys. Rev. B **47**, 7961 (1993).
- ²¹ J. Sirker, A. Klimper, and K. Hamacher, Phys. Rev. B **65**, 134409 (2002).
- ²² A. W. Sandvik and D. J. Scalapino, Phys. Rev. Lett. **72**, 2777 (1994); A. V. Chubukov and D. K. Morr, Phys. Rev. B **52**, 3521 (1995).
- ²³ D. C. Mattis, *The Theory of Magnetism I*, Springer, New York, 1981.
- ²⁴ D. N. Zubarev, Sov. Usp. Phys. **3**, 320 (1960).
- ²⁵ S. B. Haley and P. Erdős, Phys. Rev. B **5**, 1106 (1972).
- ²⁶ An exception here is the bilayer system, where isotropic magnons are obtained at $|J_c| = 2|J_{ab}|$, and then the value of δE is smaller in the *C*-AF phase than in the *A*-AF phase.
- ²⁷ G. Khaliullin, P. Horsch, and A. M. Oleś, Phys. Rev. Lett. **86**, 3879 (2001).